

Master list of "laboratory needs" prepared during a breakout session of the NASA Laboratory Physics Workshop at NASA Ames, May, 2002 (see Melissa McGrath for more details).

We would like to make a general statement of strong support for significant modeling/theoretical efforts. Many of the experiments are difficult and slow and cannot be done at all relevant temperatures and conditions. This requires good cross section calculations, simulations of molecular dynamics, etc., to enable extension of the experiments to the appropriate regimes.

Wavelength: Xray

GAS: EMISSION PROCESSES

Payoffs: Xray emission has been detected from comets, the Jovian aurora, the Io plasma torus and the Jovian Galilean satellites (Io, Europa, Ganymede). Although charge exchange has been put forward as the primary mechanism for comets, this is not widely accepted. The payoff is to understand the dominant emission process in all of these objects. If the mechanism is charge exchange for comets, it both provides a diagnostic of the comet coma composition, and samples the solar wind velocity in as many locations as measurements of bright comets can be made. The exploitation of diagnostic capabilities based on charge exchange is only in its infancy. It requires emission models that incorporate laboratory tested radiative cascade matrices and angular momentum-resolved cross sections. Future missions will return a wealth of data that will be hard to evaluate with the present state of knowledge.

Missions: Chandra; ROSAT (archival data)

Needs: Charge exchange cross sections between solar wind ion and comet coma constituents. Measurement of cross sections and rates for other proposed processes (Beiersdorfer paper at this meeting). Modeling of the emission processes.

Wavelength: UV - Visible

GAS: EMISSION PROCESSES (ATOMIC & MOLECULAR)

Payoffs: There are currently many unidentified lines from the recently observed bright comets (which include Hale-Bopp and Hyakutake) in the UV and visible wavelength ranges. Many of these are probably semi-complex parent molecules. The payoff is identification of basic compositional properties of comets, and an understanding of the complex chemistry that takes place as a comet surface is vaporized during passage through the inner solar system. Comets are considered to be one of the most pristine components left over from solar system formation, and are therefore of great interest in developing an understanding of the origin of our own solar system, and by extension, of solar systems elsewhere. Bombardment of early Earth by comets may have provided the Earth's reservoir of water, critical to the evolution of life on Earth.

Missions: FUSE; HST; ground-based observations (e.g., with NASA IRTF, Keck); CONTOUR

Needs: Enhanced UV (especially ~800-1200Å) and optical line lists for plausible parent species would be invaluable.

Wavelength: UV - radio

GAS: EMISSION PROCESSES (ATOMIC & MOLECULAR)

Payoffs: Understanding the fundamental processes (and especially especially the energy balance) associated with planetary atmospheres and magnetospheres including planetary aurora and dayglow emissions (relevant for all planets and satellites with atmospheres and magnetospheres, including the Galilean satellites and Titan). This is also relevant for comets. These studies are accomplished primarily by observing emission lines (both atomic and molecular) from these objects at all wavelengths. This work is also very relevant to the study of the Earth's atmosphere, and much of the basic atomic physics data for oxygen (important in many planetary atmospheres and magnetospheres, especially Mars, Venus, Jupiter, Io, Europa, Ganymede, Callisto, Saturn) has been motivated by research on the Earth's atmosphere.

Missions: HST, FUSE, Cassini, Galileo, Earth missions (EOS), ground-based visible, IR (including NASA IRTF and Keck), and radio observations (e.g., VLA and Arecibo); future, Pluto and Europa missions, SIRTf, SOFIA, NGST, Herschel, etc. (basically any mission that will do observations of any planet or satellite with an atmosphere, which is almost everything)

Needs: Generally speaking, reaction rates and electron impact excitation rate coefficients for the relevant species at the relevant energy. A few illustrative examples:

- Electron impact excitation of SO₂ (Venus and Io atmospheres) for relatively low electron temperature (threshold to 50eV)
- Electron impact excitation of atomic sulfur (SI) and Chlorine (ClI) resonance transitions in the FUV (~900-2000Å). They have never been measured or calculated.
- Reaction rate for CO₂(000) + O(3P) -> CO₂(010) + O(3P) (Venus, Earth, Mars).
- Energetic H/H⁺ collisions with O (Venus/Mars).
- Relaxation of O₂ excited states (Venus/Earth/Galilean satellites)
- Almost none of the charge exchange cross sections from Brown et al. (1983) and McGrath & Johnson (1987) important for modeling the energy balance and composition of the Io plasma torus and plasma in the Saturn magnetosphere have been measured experimentally.

Wavelength: UV - radio

GAS: ABSORPTION, CHEMICAL REACTIONS, COLLISION PROCESSES

Payoffs:

Determine composition and structure of planetary atmospheres and interiors. This is done primarily using the solar light reflected from the planets' atmospheres, in which absorption from the planetary atmosphere is superposed. Sounding at different wavelengths probes different depths in the planet's atmosphere. Modeling of giant planet atmospheres is also used as a basis for understanding brown dwarf atmospheres, which are very similar in many respects and have many of the same laboratory requirements particularly for species such

as methane (CH₄), carbon monoxide (CO), and water (H₂O).

Missions: HST, FUSE, CHANDRA (which detected Venus in solar reflected xray light), Cassini, Galileo, Earth missions (EOS), ground-based visible, IR (including NASA IRTF and Keck), and radio observations (e.g., VLA and Arecibo); future, Pluto and Europa missions, SIRTf, SOFIA, NGST, Herschel, etc. (basically any mission that will do observations of any planet or satellite with an atmosphere, which is almost everything)

Needs: Interpretation of such spectra requires both adequate line lists for the parent species (primarily molecular), as well as extensive sets of rate coefficients for all classes of reactions used in the photochemical models, and an understanding of the radiative transfer effects on line shapes.

It is not possible to summarize the specific needs here as they are so vast. A partial list of needs is included in Heustis et al. (2002). A few illustrative examples are given here.

- Photoabsorption, photodissociation, and photoionization cross sections (UV), photolysis branching ratios, and quantum yields for appropriate species at low temperatures. Examples:
 - Characterize CH₄ photolysis at H Lyman alpha (1215.67Å). We still do not know the photolysis branching ratios and product quantum yields. What is the relative importance of branches that produce CH₃, CH₂ and CH?
 - Measure low temperature photoabsorption and photodissociation cross sections for hydrocarbons containing from 2 to 6 carbon atoms (e.g., stable forms of C₆H₆, C₃H₄, C₃H₆, C₄H₄, and C₄H₆) at appropriate temperatures (50-100K).
 - CO₂ photoabsorption cross section (for Mars). The cross section is very structured 900-1200Å. The last measurements were in 1965 at low resolution.
 - N₂ photoabsorption cross section from 800-1000Å (minimum) at R>~100,000. The linewidth (photodissociation broadening) is also important.
 - S₂ photoabsorption cross section. S₂ has been detected in the Jovian atmosphere following in the comet Shoemaker-Levy 9 impacts, and also recently in the Pele plume in the Io atmosphere. The cross section has never been measured, and never been calculated theoretically. Crude ab initio calculations were done to provide a first superficial analysis of the existing data.
- Rate coefficients for appropriate chemical reactions at low temperatures and pressures. Examples:
 - Low-pressure limiting rate constants for many important termolecular hydrocarbon addition rates have not been obtained experimentally or theoretically (e.g., H + hydrocarbons; CH₃ + CH₃; CH₃ + C₂H_x, C₃H_x, and C₄H_x radicals; C₂H₃ or C₂H₅ + C₂H_x, C₃H_x, and C₄H_x radicals).
 - Low-temperature rate constants for important bimolecular reactions that have not been obtained or are not well constrained (e.g., H₂ + hydrocarbon radicals; CH₂ + H₂ and hydrocarbons; reactions involving C₃, C₄, C₅, and C₆ species). Information about reaction products is also critical.
- Variability of non-Lorentzian line shapes with temperature.
- Quantum or empirical ground-state potential energy surface, rovibrational energies, and transition probabilities for individual visible and near-

infrared transitions. (Giant planets and Titan)

- Equations of state, solubility, and molecular diffusion in H₂/He at low temperature and high density. (Giant planets)
- Determination of the temperature dependence of the submillimeter line wing absorption by NH₃
- Non-Lorentzian line shapes in visible, e.g., KI, that are evident in brown dwarfs and will influence the radiative transport process at depth.
- More detailed near-infrared absorption spectrum of CH₄ needed in calculating the stratospheric heating rates.
- For many of the known reactions (photodissociation rates) it is not known how the products are distributed in energy states. As a very simple example it is clear that the parent(s) of CH in comets photodissociates to produce CH in a rotationally excited state. However, the corresponding lab data do not exist, even though this might be diagnostic of the dominant parent. On the other hand, this problem is well studied for water.
- High accuracy measurements of line strengths of CO₂ and H₂O in the NIR (Mars)
- Carbon monoxide: broadening by H₂ and He (Jupiter & Saturn).
- Improved line strengths for phosphine 100-500um (Jupiter & Saturn).
- Improved line strengths and line broadening parameters for:
 - Nitriles: HCN, HC₃N, C₂N₂, CH₃CN, CH₂CHCN, and CH₃CH₂CN in the 14-50um range
 - Hydrocarbons: pure rotation lines of CH₄ near 100um (Titan); for propyne (CH₃CCH) and allene (CH₂CCH₂) improved line strengths are needed in the 12-30um region; for diacetylene (C₄H₂) the bands at 16 and 45 microns.

Wavelength: UV - radio

SOLID SURFACE PROCESSES (Sputtering, radiolysis, photolysis, synthesis of organics)

Payoffs: Fundamental understanding of solid surfaces in the solar system, especially Kuiper Belt Objects.

Missions: HST, FUSE, CHANDRA (which detected Venus in solar reflected xray light), Cassini, Galileo, Earth missions (EOS), CONTOUR, STARDUST, MESSENGER, NEAR, DAWN, all the MARS missions, ground-based visible, IR (including NASA IRTF and Keck), and radio/radar observations (e.g., VLA and Arecibo); future, Pluto and Europa missions, SIRTIF, SOFIA, NGST, Herschel, etc. (basically any mission that will do observations of any planet or satellite without a substantial atmosphere that inhibits study of the surface, which is almost every mission that NASA does).

Needs:

- Reflectance spectra (UV-visible-NIR) of low temperature frosts/volatile ices. There is currently a big hole in the temperature range 50-150K.

Water is reasonably well covered, and the mid- and far-IR has been done for astrophysical ices, although not at the temperatures relevant for solar system objects. Lack of these data have inhibited interpretation of the Galileo data. Unless something is done in the near future the situation will be similar for Saturn Cassini data.

- Optical constants/properties of organic solids (important for most "red" solid bodies in the outer solar system including Titan, Kuiper Belt Objects, Triton, Pluto, Charon, etc.).
- Properties of solid sulfur (S₂ - S₈). (Important for Io).
- To understand the processed "goop" that makes KBOs dark and reddish (or neutral as the case may be). This includes irradiation experiments to simulate long-term exposure to cosmic rays. The experiments need to produce results observers can use (e.g., optical-IR spectra).
- Low velocity collisions of icy dirt balls have direct relevance to the Kuiper Belt.
- Mechanical properties of cryogenic porous ice/rock aggregates. The applications include Kuiper Belt Objects and the outer planet satellites, many of which also have densities near 1000 kg/m³ and so which are likely to be porous.
- G-values (yield per 100eV desposited) for pure and mixed ices relevant to the icy satellites, Kuiper Belt Objects, etc., are extremely sparse. They depend on T, irradiation time, particle type and velocity. For example, for OH or peroxide trapped in ice, the classic experimental results have been shown to be incorrect because of unknown contaminants. One needs to do these experiments as a controlled function of known impurities and T. Sputtering yields are also still problematic because the materials of interest have chemical effects that depend on temperature, and therefore certainly also contaminants. This will be critical for the Saturn system science (Cassini).
- The sputter produced O₂ relevant for the atmospheres of icy satellites (e.g., Europa, Ganymede, Saturn icy satellites) is very poorly known for the right ions, energies, temperatures and contaminants. All modeling requires more O₂ than has been measured so far.
- Studies of thermal and photon stimulated desorption are important for many solid surfaces in the solar system, especially porous regoliths where sticking to neighboring grains is relevant.
- Visible through thermal IR lab spectroscopy of minerals, mineral mixtures (terrestrial analogs) and ices relevant to Mars over a wide range of particle sizes and viewing geometries. FOr example, interpretations of the Mars Global Surveyor/Thermal Emission Spectrometer spectra continue to rely on a small set of lab mineral spectra of primarily coarse-grained ineral smaples, while there is much evidence that most of the materials on Mars are extremely fine-grained or perhaps even amorphous. The limitations on the available lab data will also hamper interpretations of thermal IR spectra to be obtained from the surface in 2004 by the Mars Exploration Rovers. The situation is similar in the visible to NIR, which will be studied extensively at the tens of meters scale by a NIR spectrometer on the 2005 Mars Reconnaissance Orbiter mission.

- Laboratory geochemical studies of Martian surface and interior petrology and geochemistry. These studies focus on trying to match the remote sensing, in situ, or SNC meteorite measurements of surface chemistry and mineralogy by running experiments on magma partitioning under martian conditions, surface UV irradiation reactions, surface hydration/dehydration and adsorptivity studies (Mars water cycle), and studies of heterogeneous chemistry occurring on and in dust grains as catalysts for atmospheric photochemistry.
- Better dielectric measurements of a variety of martian materials (UV through IR) are needed.